Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Highly efficient orange and deep-red organic light emitting diodes with long operational lifetime using carbazole-quinoline based bipolar host materials

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Synthesis of 9-(4-(4-(4-Bromophenyl)quinolin-2-yl)phenyl)-9*H*-carbazole (CzPPQBr):

A mixture of 1-(4-(9*H*-carbazol-9-yl)phenyl)ethanone (285 mg, 1.00 mmol), (2-aminophenyl)(4-bromophenyl)methanone (553 mg, 2.00 mmol), diphenyl phosphate (751 mg, 3.00 mmol), and freshly distilled *m*-cresol (1.0 mL) was heated under nitrogen at 140 °C for 12 h. After cooling, the reaction mixture was added to a solution of 10% (v/v) triethylamine in methanol (10.0 mL). The precipitated product was purified by column chromatography (hexane/EtOAc, 10:1) to yield **CzPPQBr** (426 mg, 81.2%). ^{1}H NMR (400 MHz, $CDCl_3$, δ):7.30 (dd, 2H, *J* = 7.2, 7.2 Hz), 7.40-7.52 (m, 7H), 7.69-7.80 (m, 7H), 7.86-7.88 (m, 2H), 8.14 (d, 2H, *J* = 7.2 Hz), 8.27 (d, 1H, *J* = 8.8 Hz), 8.41 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, δ): 109.8, 119.0, 120.1, 120.4, 122.9, 123.6, 125.3, 125.5, 126.0, 126.8, 127.3, 129.1, 129.9, 130.3, 131.2, 131.9, 137.2, 138.4, 138.9, 140.7, 148.2, 148.9, 156.0; HRMS (EI, m/z): [M^+] calcd for $C_{33}H_{21}BrN_2$, 524.0888; found, 524.0893.

Synthesis of 9-(4-(6-Bromo-4-phenylquinolin-2-yl)phenyl)-9*H*-carbazole (CzPPBrQ):

A mixture of 1-(4-(9*H*-carbazol-9-yl)phenyl)ethanone (285 mg, 1.00 mmol), (2-amino-5-bromophenyl)(phenyl)methanone (553 mg, 2.00 mmol), diphenyl phosphate (751 mg, 3.00 mmol) and freshly distilled *m*-cresol (1.0 mL) was heated under nitrogen at 140 °C for 12 h. After cooling, the reaction mixture was added to a solution of 10% (v/v) triethylamine in methanol (10.0 mL). The precipitated product was purified by column chromatography (hexane/EtOAc, 10:1) to yield **CzPPBrQ** (437 mg, 83.2%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.30 (ddd, 2H, *J* = 8.0, 7.6, 1.0 Hz), 7.42 (ddd, 2H, *J* = 8.0, 6.8, 1.2 Hz), 7.48-7.50 (m, 2H), 7.55-7.60 (m, 5H), 7.73 (d, 2H, *J* = 8.4 Hz), 7.82 (dd, 1H, *J* = 9.0, 6.2 Hz), 7.91 (s, 1H), 8.07 (d, 1H, *J* = 3.0 Hz), 8.13-8.16 (m, 3H), 8.41 (d, 2H, *J* = 8.4 Hz); ^{13}C NMR (100 MHz, $CDCl_3$, δ): 109.7, 109.8, 119.9, 120.2, 120.4, 120.7, 123.6, 126.4, 127.1, 127.3, 127.9, 128.8, 128.9, 129.1, 129.4, 131.8, 133.3, 137.6, 138.0, 139.1, 140.6, 148.8, 156.2; HRMS (EI, m/z): [M^+] calcd for $C_{33}H_{21}BrN_2$, 524.0888; found, 524.0897.

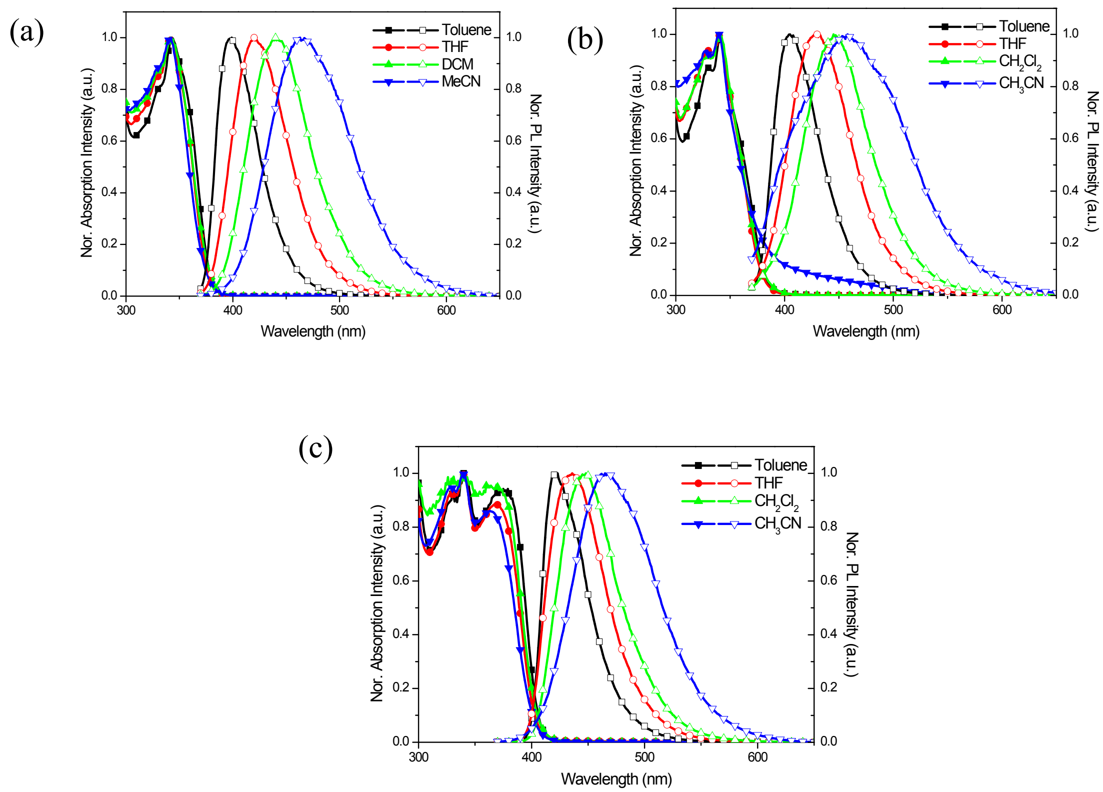


Fig. S1 The absorption and photoluminescence spectra of (a) **CzPPQ**, (b) **CzPPCzQ**, and (c) **CzPPCzQ** in toluene, tetrahydrofuran, dichloromethane and acetonitrile solution (10^{-4} M).

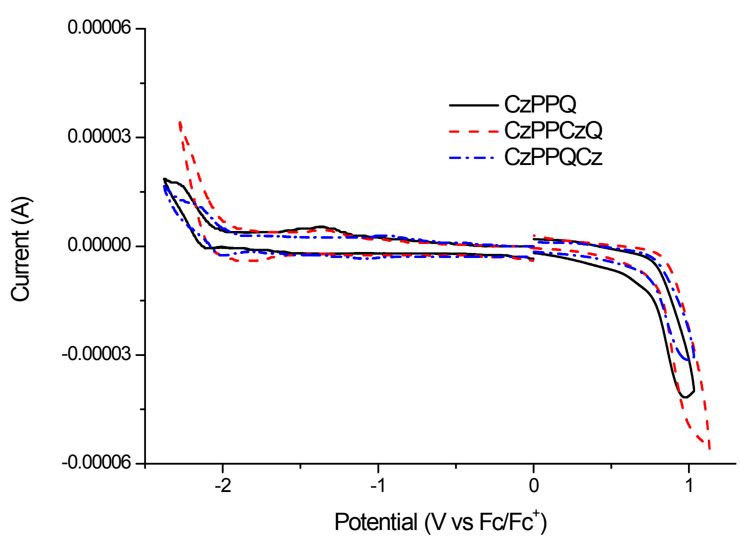
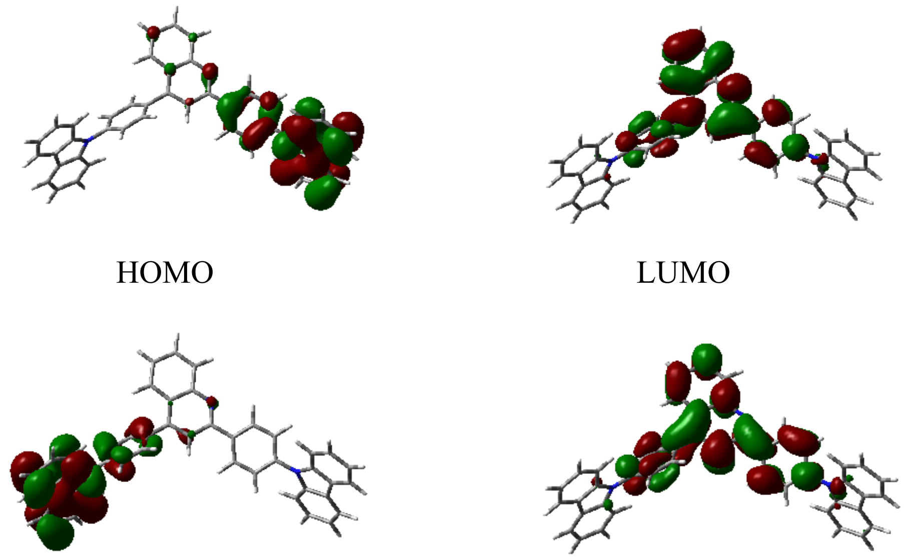


Fig. S2 Cyclic voltammetry measurement of **CzPPQ**, **CzPPCzQ** and **CzPPQCz.**

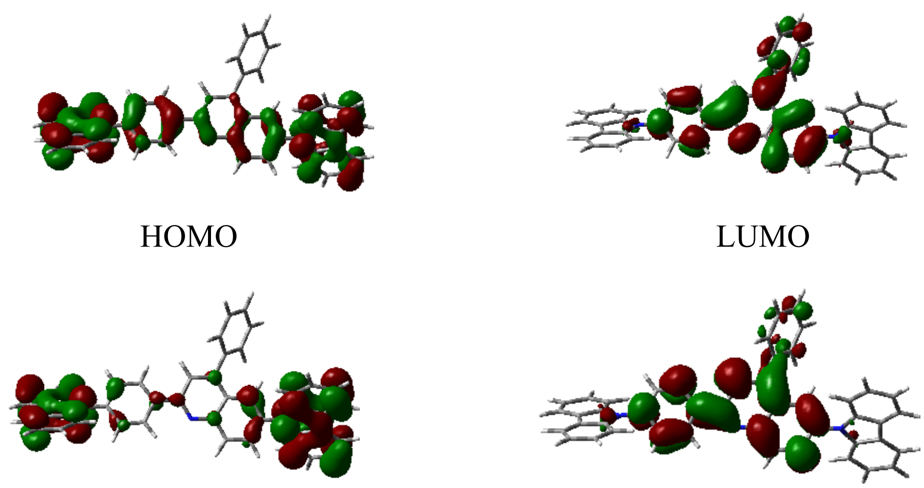
(a) **CzPPCzQ**



HOMO LUMO

HOMO-1 LUMO+1

(b) **CzPPQCz**



HOMO LUMO

HOMO-1 LUMO+1

Fig. S3 Calculated electron contour plots of the occupied and unoccupied molecular orbitals of (a) **CzPPCzQ** and (b) **CzPPQCz**

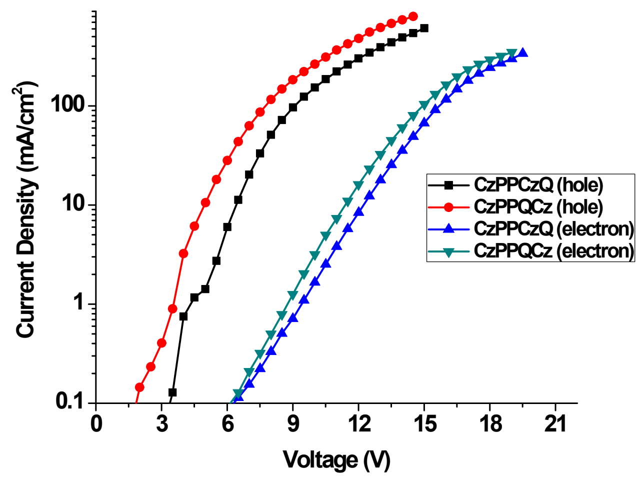


Fig. S4 Current density versus voltage for the hole-only and electron-only devices of **CzPPCzQ** and **CzPPQCz**.

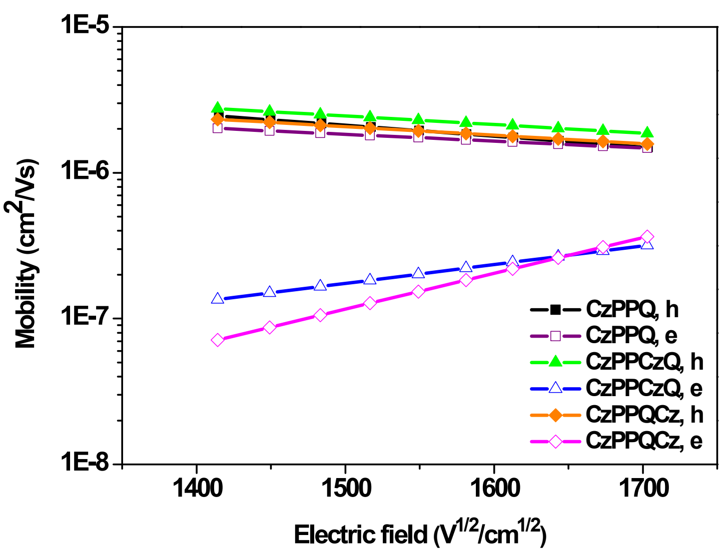


Fig. S5 The relationship of hole and electron mobility vs the electric field. The mobilities of CzPPQ, CzPPCzQ and CzPPQCz were determined by SCLC method. Device structure: ITO/ MoO_3 (1)/ CzPPQ or CzPPCzQ or CzPPQCz (50)/ MoO_3 (10)/Al (100) for hole only and ITO/ Ca (5)/ CzPPQ or CzPPCzQ or CzPPQCz (50)/ Ca (5)/Al (100) for electron only.

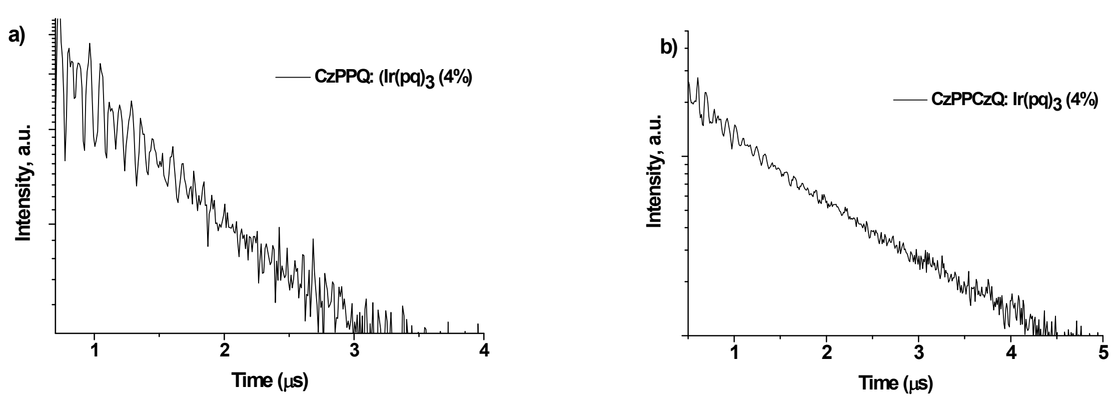
Table S1. Hole and electron mobility of host materials.

Materials	hole mobility (cm^2/Vs)^a	electron mobility (cm^2/Vs)^a
CzPPQ	2.13x10^{-6}	1.81x10^{-6}
CzPPCzQ	2.43x10^{-6}	1.16x10^{-7}
CzPPQCz	2.09x10^{-6}	1.70x10^{-7}

^{a}Mobility value at 1500 (V/cm)$^{1/2}$

Table S2. Phosphorescence lifetime of Ir(piq)$_3$ and Ir(piq)$_3$ co-deposited with **CzPPQ**, **CzPPCzQ** and **CzPPQCz**

Dopants	Host	τ (μs)
Ir(pq)$_3$	CzPPQ	1.41
Ir(pq)$_3$	CzPPCzQ	1.06
Ir(pq)$_3$	CzPPQCz	1.03
Ir(piq)$_3$	CzPPQ	1.18
Ir(piq)$_3$	CzPPCzQ	1.04
Ir(piq)$_3$	CzPPQCz	0.98



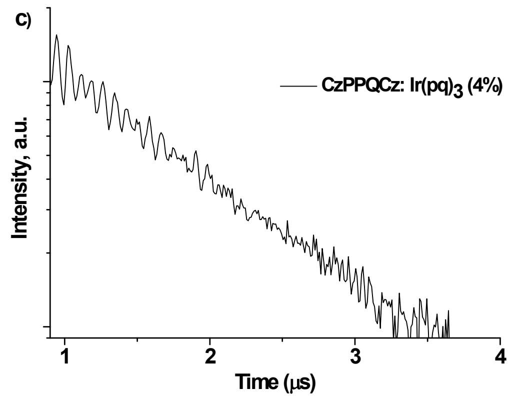


Fig S6. Transient PL decay for 4 wt.% $Ir(pq)_3$-doped a) **CzPPQ**, b) **CzPPCzQ** and c) **CzPPQCz** thinfilms.

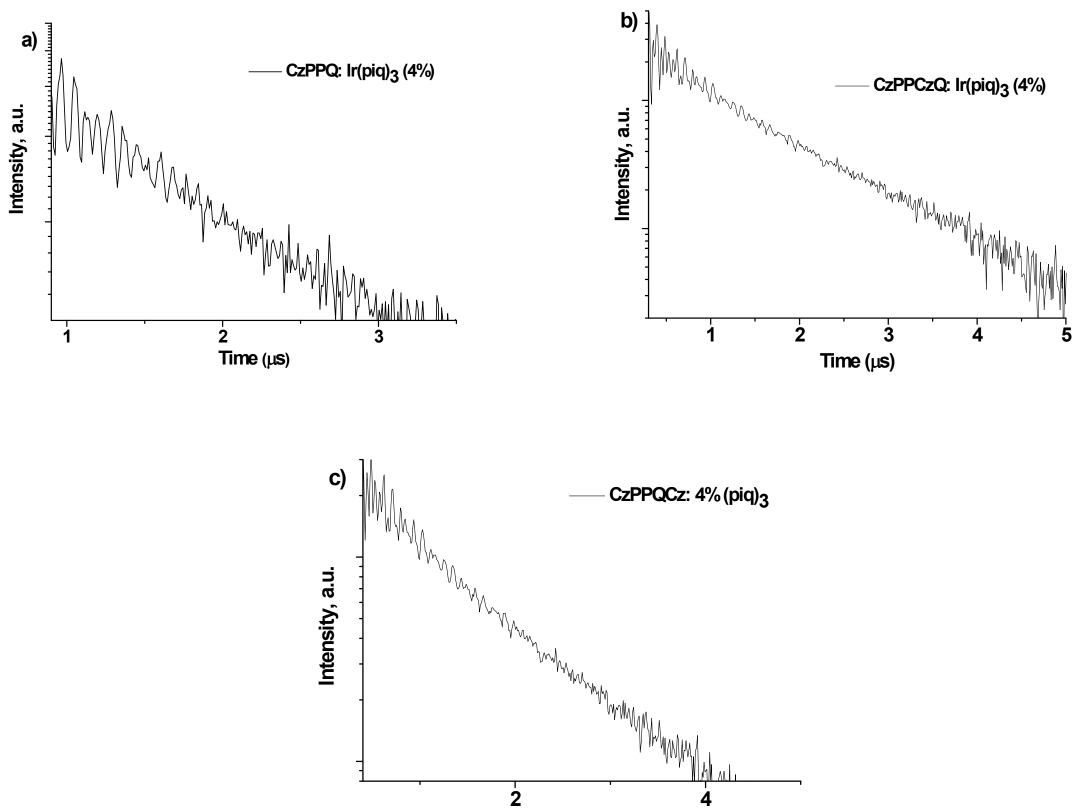


Fig S7. Transient PL decay for 4 wt.% $Ir(piq)_3$-doped a) **CzPPQ**, b) **CzPPCzQ** and c) **CzPPQCz** thinfilms.

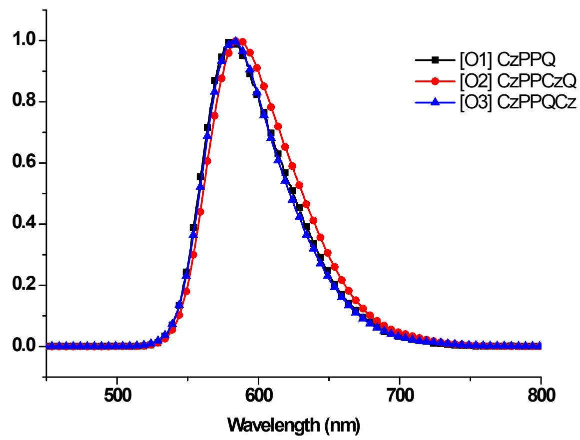


Fig. S8 Electroluminescence spectra of devices O1-O3 at 8V

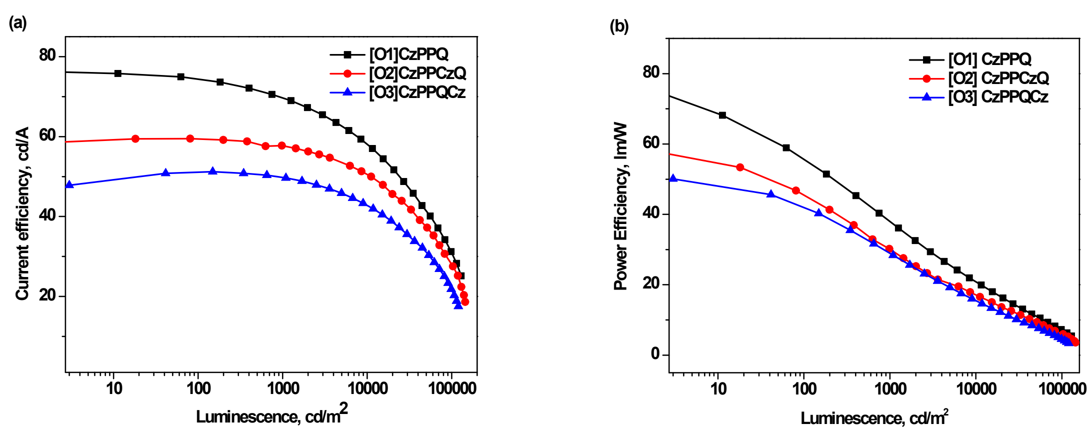


Fig. S9 (a) Luminescence vs current efficiency and (b) Luminescence vs power efficiency curves of devices O1-O3

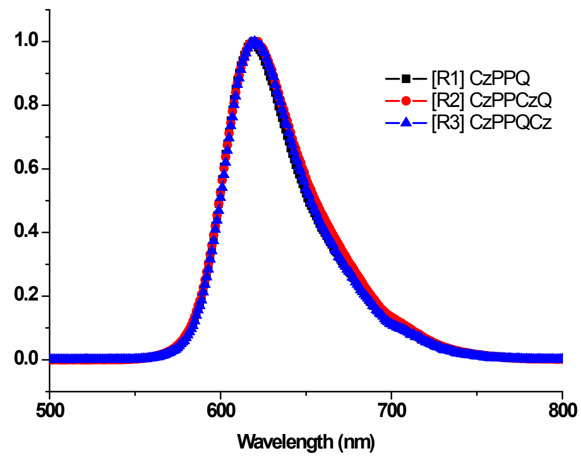


Fig. S10 Electroluminescence spectra of R1-R3 devices at 8V